NEMD Simulations of Metallic Friction

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Abstract

The properties of metal interfaces sliding at high velocities under strong compression have been studied using Non Equilibrium Molecular Dynamics (NEMD). The systems studied include model Lennard-Jones systems and systems modeled more realistically with Embedded Atom Method (EAM) many-body potentials. These latter include Cu/Cu, Cu/Ag, and Al/Ta tribo-pairs. We discuss the nature of these simulations in terms of the underlying physical mechanisms responsible for some of the generic behavior seen in the pressure and velocity dependence of the tangential force. An analysis of the low and high velocity behavior is presented in terms of linear response theory at low velocities and a model of structural transformation at high velocities. Emphasis will be given to Al/Ta interfaces where experimental data is expected from dynamic experiments at the Los Alamos ATLAS pulsed power facility.

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- At moderately compressed sliding interfaces for dry sliding there is evidence form experiment and simulations that the formation of micro= and nano-structure is involved (D.A.Rigney and J.E. Hammerberg, MRS Bull. **23**,32-36 (1998)).

- For weakly coupled interfaces linear response with phonon damping can describe dissipation:

$$F_{12} = \frac{2\pi}{\Omega}\sum_{\vec{q}}\left(\vec{q}\cdot\frac{\vec{v}_r}{|\vec{v}_r|}\right)\left|\phi_{12}(\vec{q})\right|^2\int d\omega\left(S_1(\vec{-q},\vec{q};\omega)\mathrm{Im}G_2^{ret}(\vec{q},-\vec{q};\omega_0(\vec{q})-\omega)\right.$$

$$\left. + S_2(\vec{q},\vec{-q};\omega)\mathrm{Im}G_1^{ret}(\vec{q},-\vec{q};\omega_0(\vec{q})-\omega)\right)$$

$$\omega_0(\vec{q}) = \vec{q}\cdot\vec{v}_r$$

- For strongly coupled interfaces more complex phenomena are important:

  dislocation dynamics and nucleation

  micro- and nano-structure formation

  mechanical material mixing and alloying

- We are investigate some of these questions using large scale MD simulations in 3D and present results for Ta/Al and Cu/Ag interfaces.

Potentials

- We use EAM potentials since we believe that these are necessary in modeling locally non-uniform systems with dislocations.
- Cu/Ag: Voter EAM potentials
- Ta/Al: New Ta and Ta-Al potentials using standard EAM Methods (Daw and Baskes, PRL **50**, 1285(1993); A.F.Voter, in Intermetallic Compounds, (Wiley, 1993))

$$E = \sum_i \left(F_i(\rho_i) + \frac{1}{2} \sum_{j \neq i} \phi_{ij}(r_{ij}) \right),$$

ρ_i: electron density at i due to atoms within a cutoff radius r_{max}

ϕ_{ij}: pair potential

$F_i(\rho_i)$: embedding energy

$$\rho_i = \sum_{j \neq i} f_j(r_{ij}).$$

Fitting procedure:

$\phi = \phi_{Morse}$ for Ta, Al

$$\phi = c_1 \left[(1 - e^{-c_2(r - c_3)})^2 - 1 \right].$$

Electron density for Al from (Chen et al., J. Mater. Res **4**, 62(1989))

$$\rho_{Al}(r) = c_4 r^6 [e^{-c_5 r} + 2^9 e^{-c_5 r}].$$

Fitting parameters for Al in (Angelo et al., Model. Simul. Mater. Sci. Eng. **3**,289 (1995), Baskes et al., Model. Simul. Mater. Sci. Eng. **5**, 651(1997))

For Ta a more general form of electron density was used:

$$\rho_{Ta}(r) = c_4 \left[e^{-c_5 r} + c_6 r^{c_7} e^{-2c_8 r} \right].$$

(c_4 doesn't affect the properties of the pure material, but does allow for the scaling properties of an alloy system.)

The embedding function $F(\rho)$ is obtained from the EOS of each element in its equilibrium structure (Ta:bcc, Al:fcc)

$$F(\rho) = E_R - \frac{1}{2} \sum_{j \neq i} \phi(r_{ij}).$$

E_R is Rose's EOS (J.H. Rose et al., PRB **29**, 2963(1984))

$$E_R(V) = -E_c[1 + \hat{a} + b^3 \hat{a}^3 + b_4 \hat{a}^4] e^{-\hat{a}},$$

E_c: cohesive energy

a_0: lattice constant

B: bulk modulus

Ω: equilibrium volume

The pair potential and electron density are cut off smoothly at $r=r_{max}$ using

$$f_{cut}(r) = \begin{cases} 1 & (r < r_s) \\ \left(1 - \left(\frac{r - r_s}{r_{max} - r_s}\right)^3\right)^3 & (r_s < r < r_{max}) \\ 0 & (r > r_{max}) \end{cases}.$$

Parameters:

b_3, b_4 from Strachan et al.,2002

Data used to fit EAM Ta:

Zero pressure elastic constants (Cynn and Yoo, PRB **59**, 8526(1999))

Vacancy formation energy

Unrelaxed surface energy

Differences in E_{fcc}/E_{bcc} from first principles calculations (Söderlind and Moriarty, PRB **57**, 10340(1998))

Ta Fitting Parameters

Quantity	Value	Units
E_c	8.1	eV/atom
Ω	18.04	$Å^3$/atom
α	4.93445	
b_3	$-7.178\ 10^{-3}$	
b_4	$5.04\ 10^{-6}$	
c_1	10.39159	eV
c_2	1.793339	$Å^{-1}$
c_3	2.448770	Å
c_4	0.180370	
c_5	7.855023	$Å^{-1}$
c_6	3.674214	
c_7	12.645554	
c_8	5.8957811	$Å^{-1}$

Ta Fitting Parameters

Quantity	Value	Units
r_s	2.7632600	Å
r_{max}	5.0755330	Å

Ta-Al pair potential same as for Al, Ta and the cross potential truncated to the same r_{max} as Ta.

Potential fit to:

Heat of formation and equilibrium volume of Ta_3Al and Al_3Ta (Subramanian et al., Metall. Trans. **21A**, 539(1990).

Ta-Al fitting parameters

Quantity	Value	Units
c_1	4.7640143	eV
c_2	1.1446628	$Å^{-1}$
c_3	1.4123214	Å
r_s	4.1420358	Å
r_{max}	4.7689902	Å

Ta/Al Alloys

Alloy	ΔH (eV/atom)	E_c (eV/atom)	Ω ($Å^{-3}$/ atom)
Ta_3Al	-0.045	-6.96	15.51
	(-0.0965)	(-7.01)	17.69
Al_3Ta	-0.275	-4.82	14.506
	(-0.2464)	(-4.79)	(15.79)

Ta-Ta elastic constants

(In units: $eV/Å^3$)

c_{11}	c_{12}	c_{44}	G_s	B
1.647	0.9987	0.5167	0.19128	1.2147
(1.6474)	(0.9984)	(0.5117)	(0.194)	(1.2147)

Simulation Methodology

- F_{tang} applied uniformly in reservoir region so that $\langle v_{tang} \rangle_{res} = \pm u_p$.
- System size: 5.5 10^6 atoms
- Equilibration at initial volumes appropriate to P_0=Load/Area for 12 t_0 followed by a uniform step function velocity profile.
- Thermostatting in the reservoir regions (20 lattice planes thick)

Configurations

Cu/Ag: (100) on (100) sliding in <100>

P= 5.1 GPa

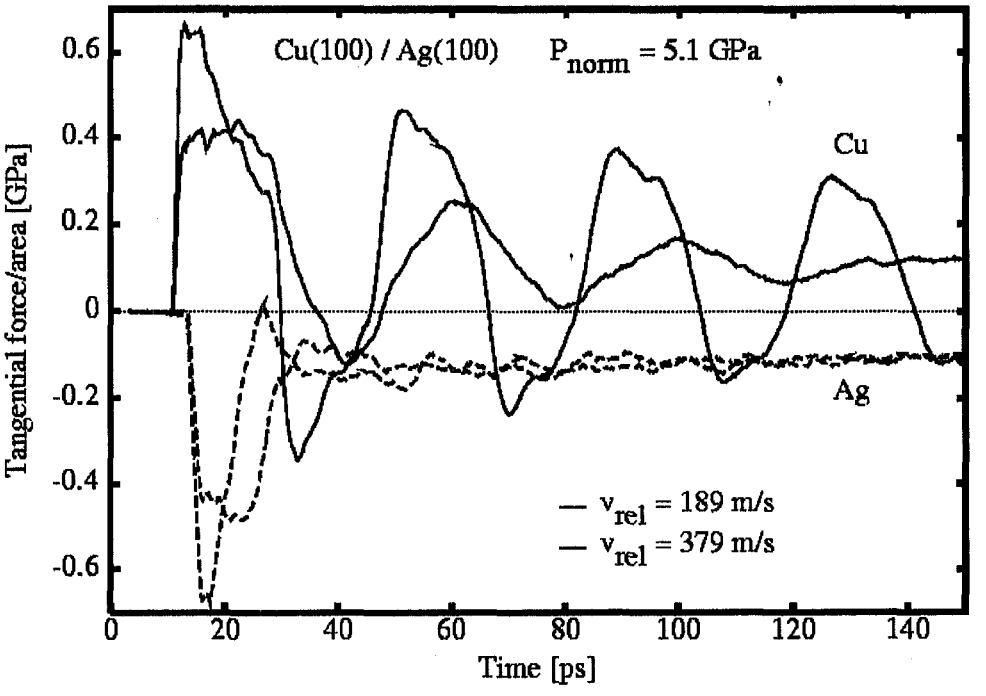
v_{tang}=189 m/s; 379 m/s

Ta/Al: (100) on (100) sliding in <100>

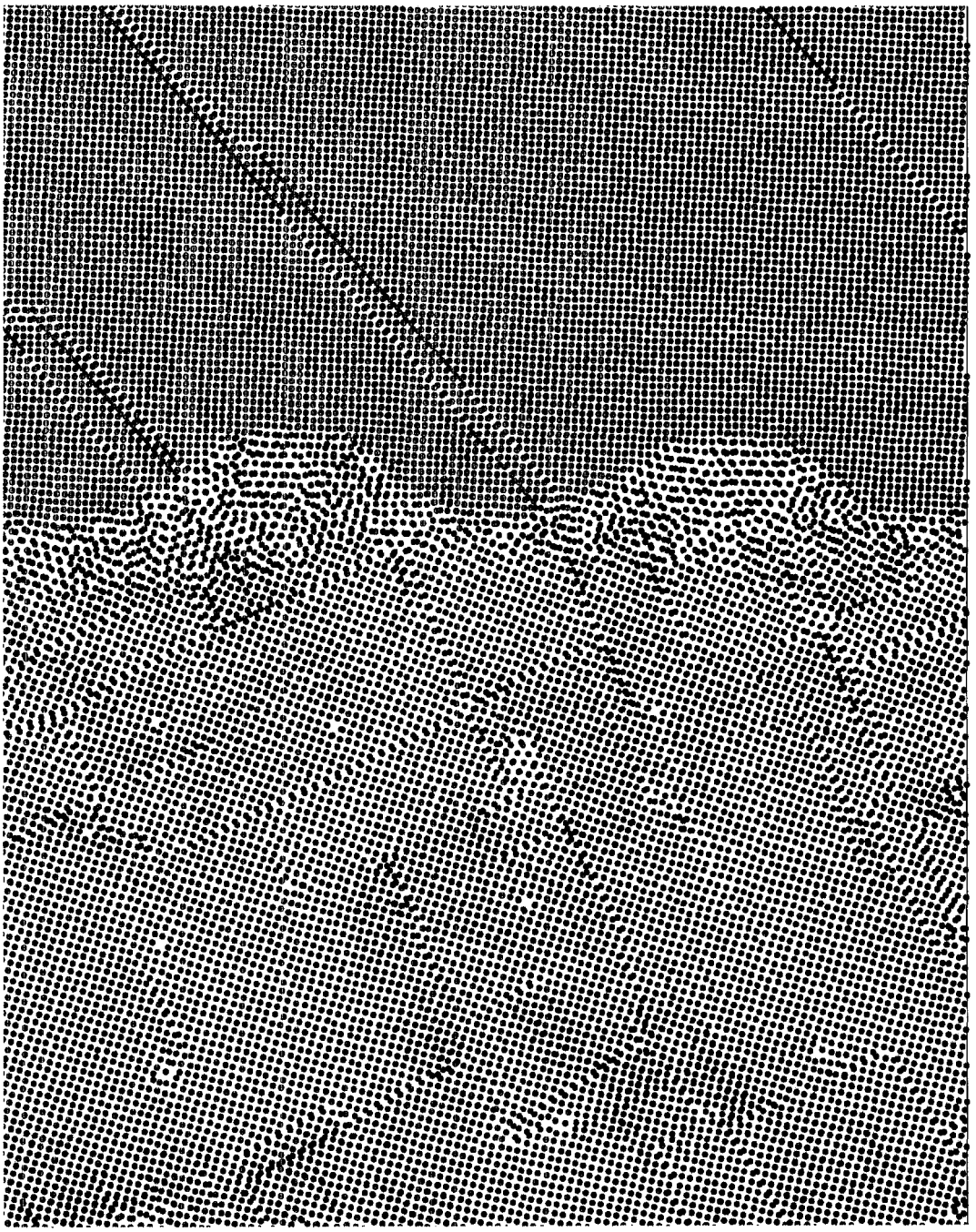
P= 17.0 GPa

v_{tang}=600 m/s

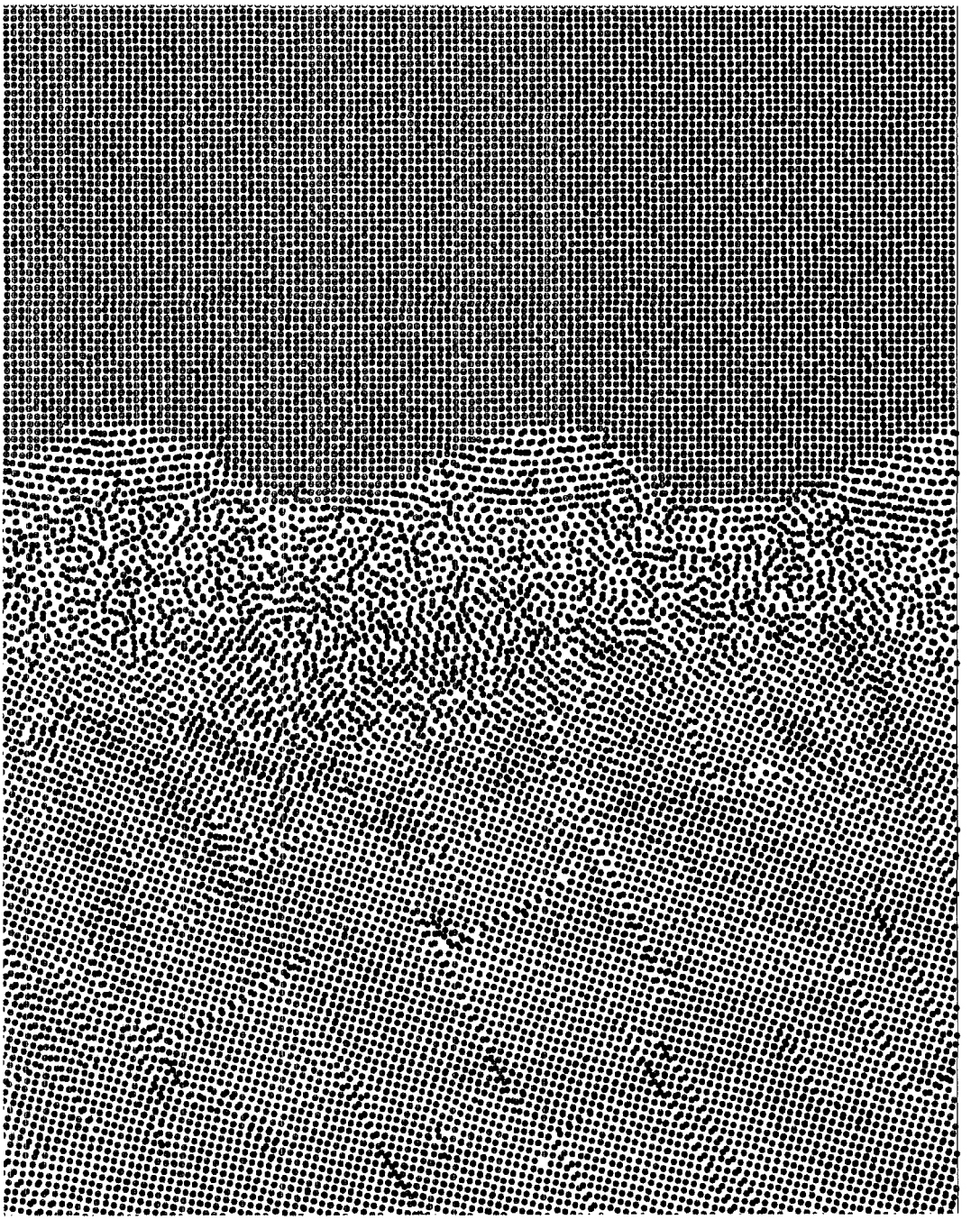
Results



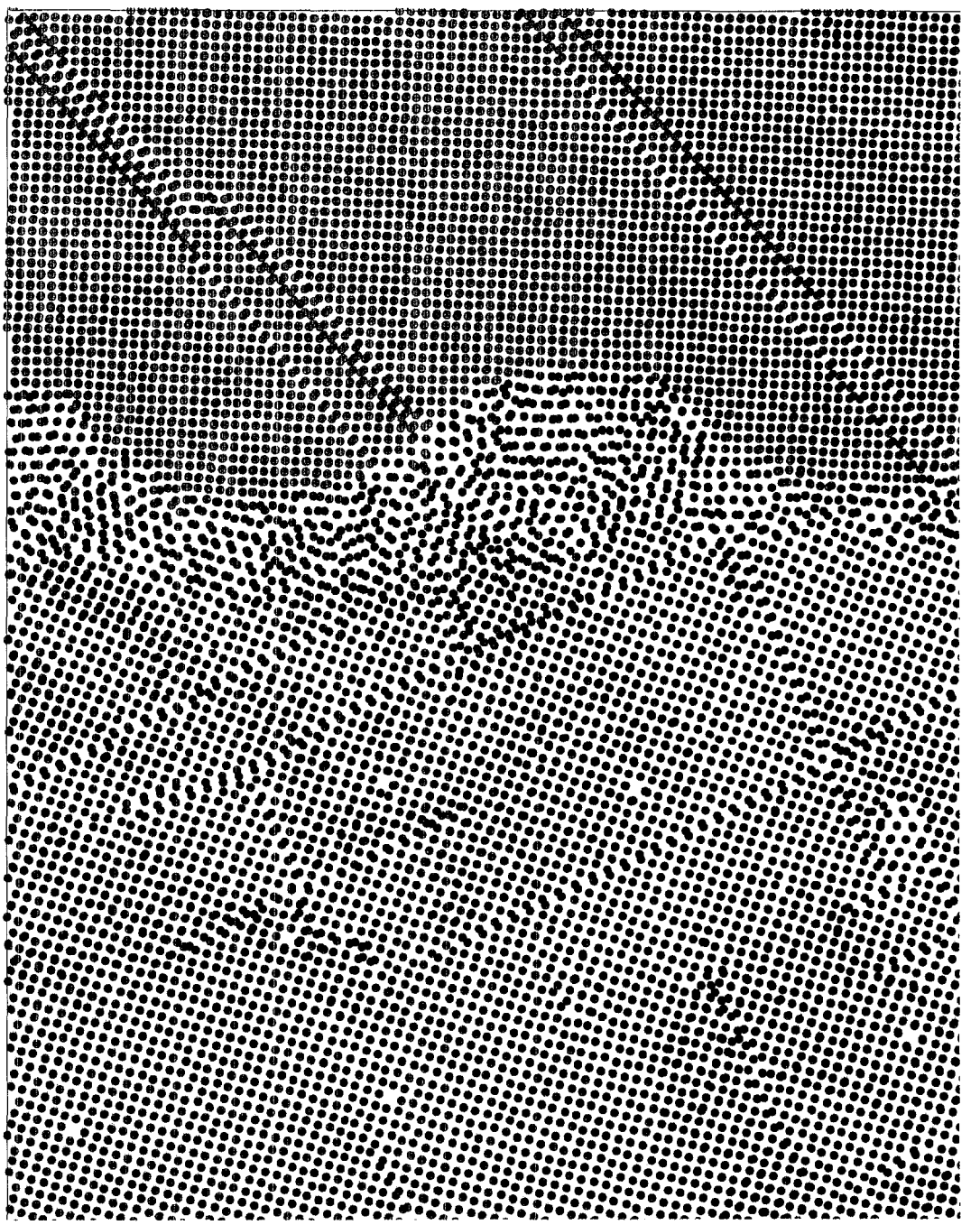
F_{tang} vs. time for Cu/Ag



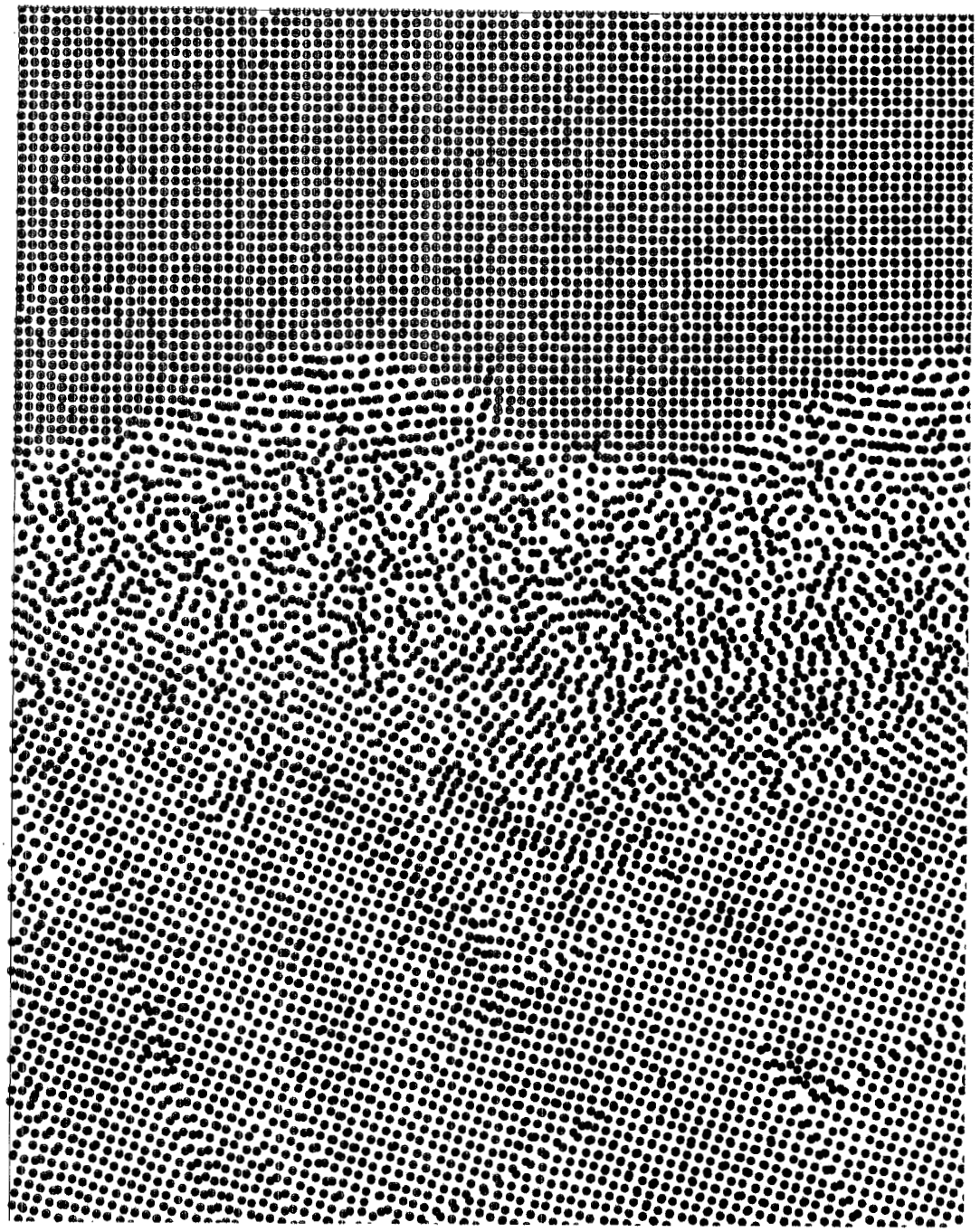
Slice along <100>, v_{tang}=189 m/s, Cu above



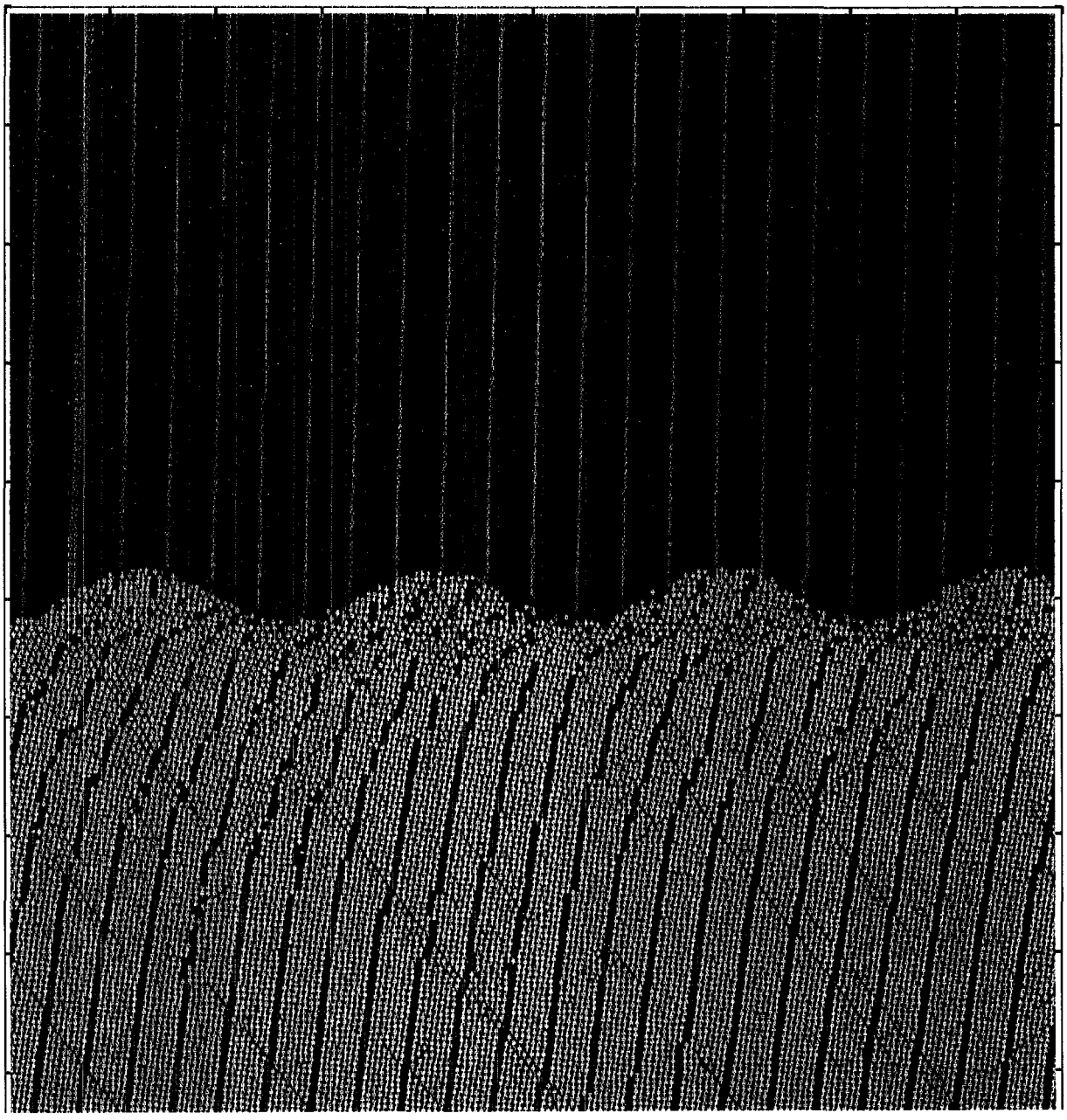
Slice along <100>, v_{tang}=379 m/s, Cu above



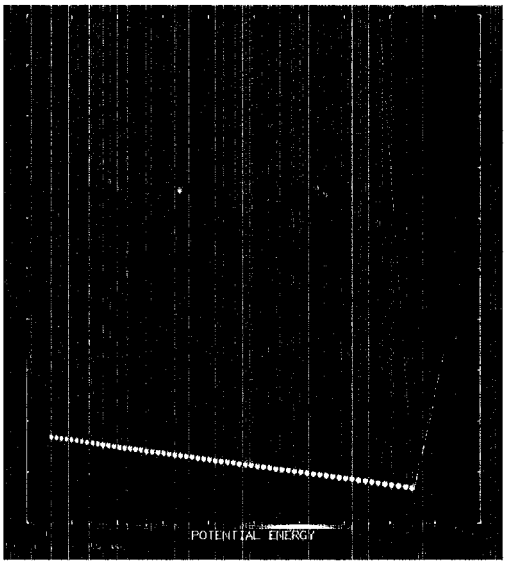
Slice along <100>, v_{tang}=189 m/s, Cu above



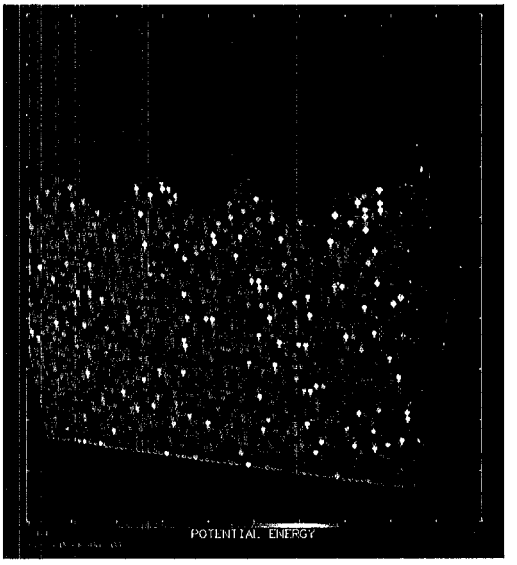
Slice along <100>, v_{tang}=379 m/s, Cu above



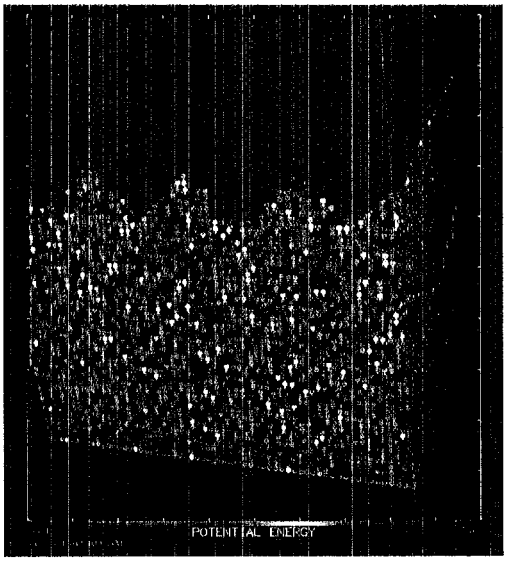
Slice along <100>, v_{tang}=189 m/s, Cu above



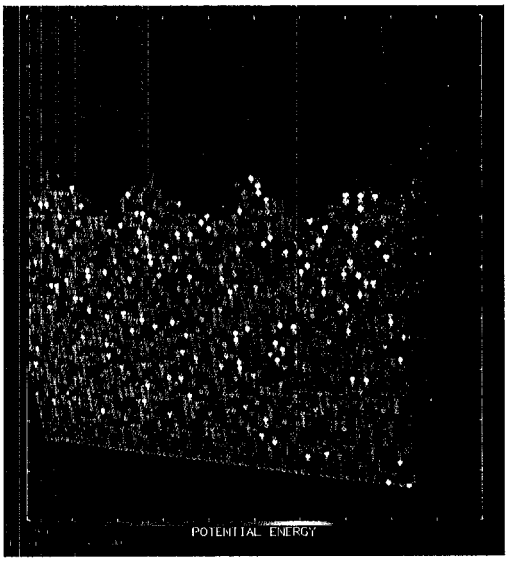
t=0



t=76 ps



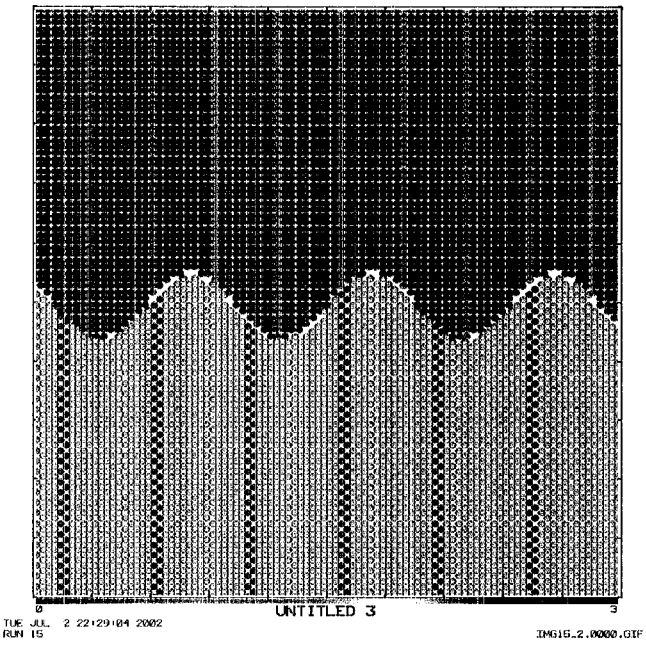
t=153 ps



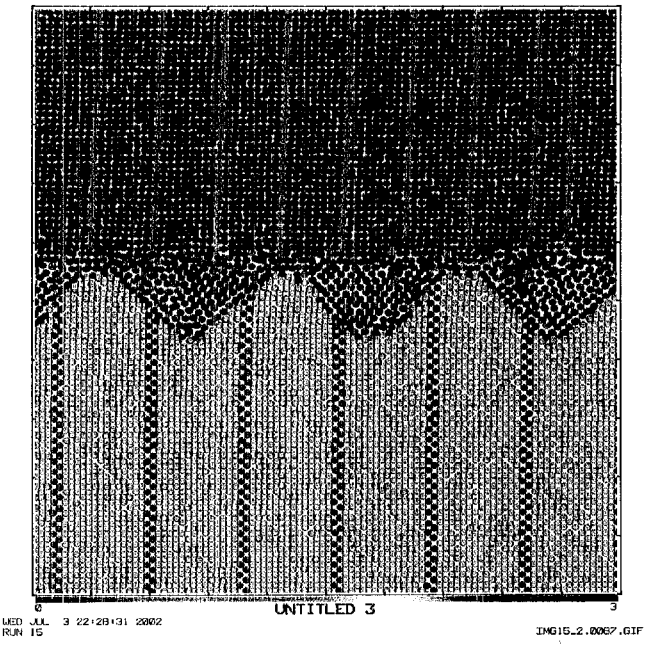
t=220ps

Ta/Al. P=17GPa, v=600 m/s

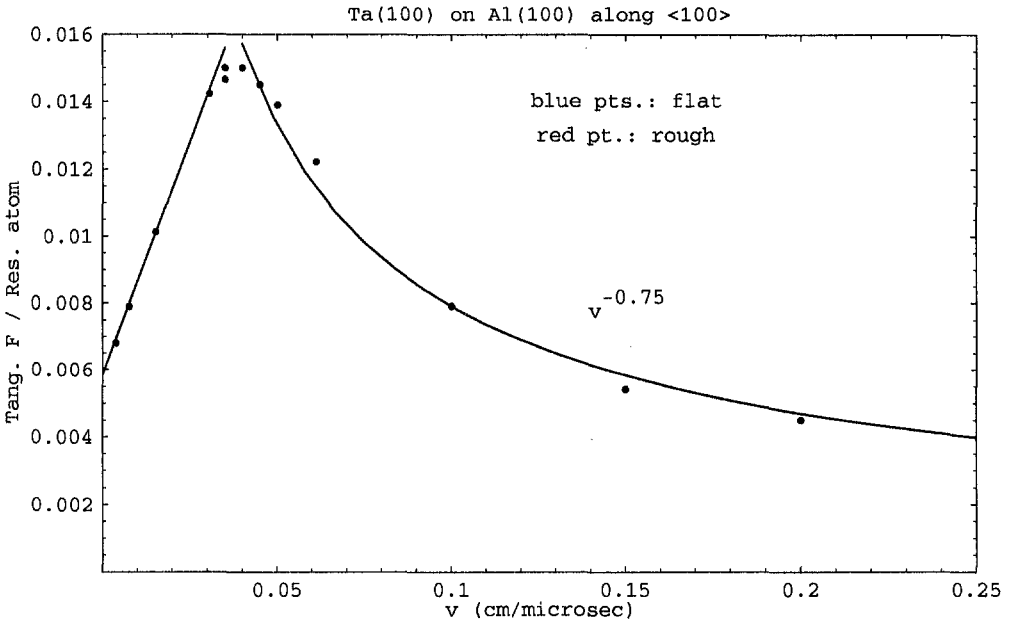
(Al above, Ta below)

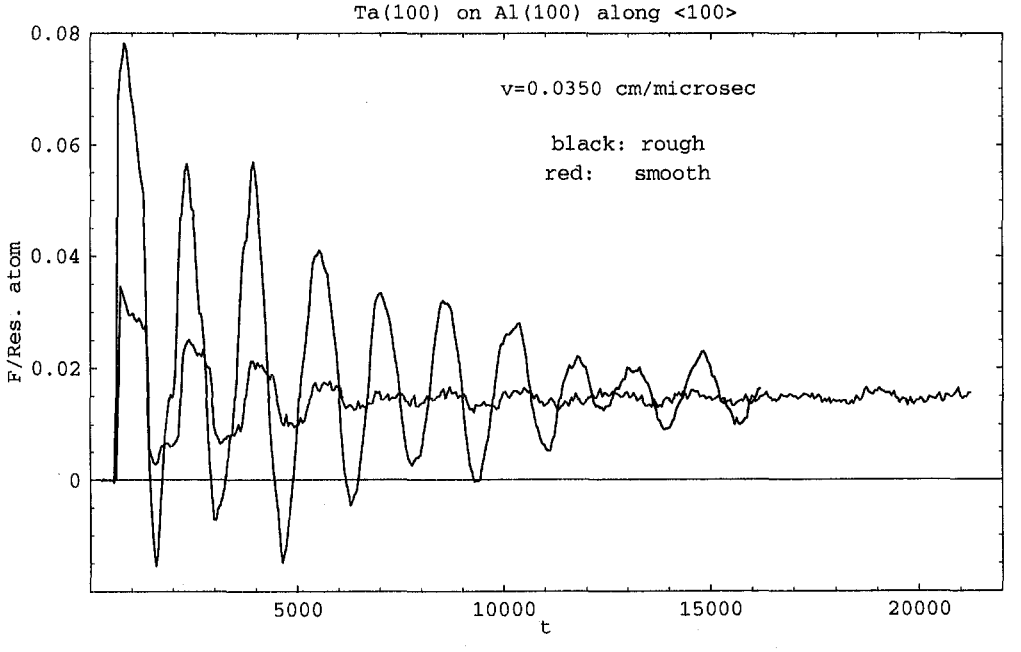


Ta/Al P=17 Gpa, t=0



Ta/Al, P=17 GPa, t=220 ps


Ta(100) on Al(100) along <100>
blue pts.: flat
red pt.: rough
v^-0.75
Tang. F / Res. atom
v (cm/microsec)
0.016
0.014
0.012
0.01
0.008
0.006
0.004
0.002
0.05
0.1
0.15
0.2
0.25


Ta(100) on Al(100) along <100>
v=0.0350 cm/microsec
black: rough
red: smooth
F/Res. atom
t
0.08
0.06
0.04
0.02
0
5000
10000
15000
20000

Summary

- In the Cu/Ag pair, the weaker Ag is strongly deformed relative to the weaker Cu.
- In the weakly corrugated interface we have studied the weaker Ag flows plastically and is entrained in the stronger Cu valleys.
- The underlying structure in the Ag is refined away from the interface with very small scale structure near the interface followed by faulted regions farther away.
- The apparent length scales are smaller at the higher velocities.
- At the converged 189 m/s velocity for Cu/Ag, $F_{tang}/A = 0.1GPa$ and $\mu=0.02$
- For Ta/Al we have to date considered only the (100) interface sliding along <100> at 17Gpa and v=600 m/s.

- The Al is entrained with the potentials we have used.
- The high velocity behavior is consistent with a power law in v, $F_{tang} \sim v^{-3/4}$ which is essentially the same behavior observed previously for 2 dimensional Lennard-Jones systems and is consistent with arguments relating microstructure formation to the high rate limit of the plastic flow stress.
- For the Ta/Al case current experiments are underway at the Los Alamos ATLAS pulsed power facility to test some of the theoretical ideas and simulations discussed here.